

Supplementary information

Exotic stable cesium polynitrides at high pressures

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Supplementary Figures

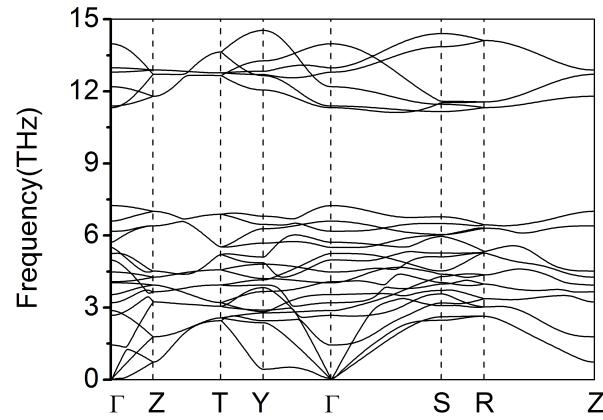


Fig. S1. Phonon dispersion curves of Cs₃N in the *Cmcm* phase at 50 GPa. The absence of any imaginary frequency in the whole Brillouin zone demonstrated that *Cmcm* structure of Cs₃N is dynamically stable.

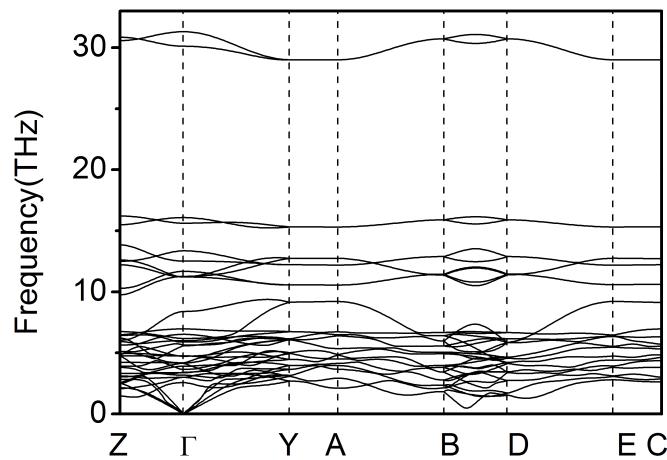


Fig. S2. Phonon dispersion curves of Cs₂N in the *C2/m* phase at 50 GPa. The absence of any imaginary frequency in the whole Brillouin zone demonstrated that *C2/m* structure of Cs₂N is dynamically stable.

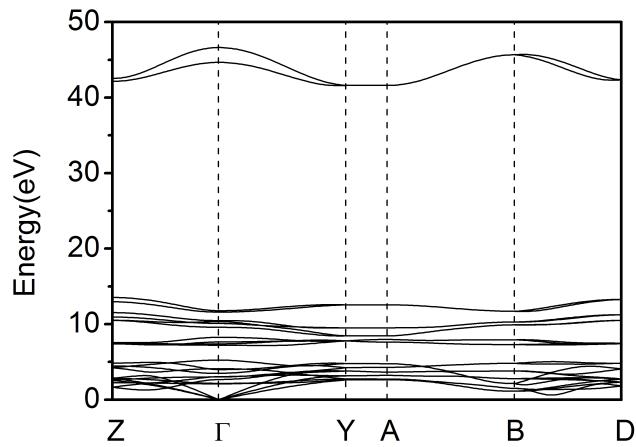


Fig. S3. Phonon dispersion curves of CsN in the $C2/m$ phase at 20 GPa. The absence of any imaginary frequency in the whole Brillouin zone demonstrated that $C2/m$ structure of CsN is dynamically stable.

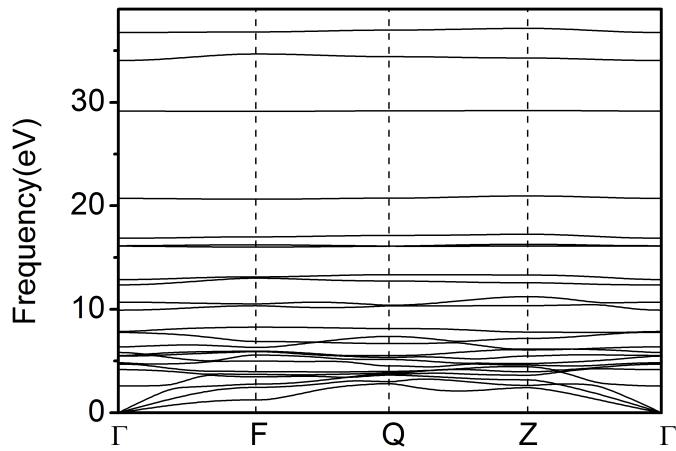


Fig. S4. Phonon dispersion curves of CsN in the $P-1$ phase at 50 GPa. The absence of any imaginary frequency in the whole Brillouin zone demonstrated that $P-1$ structure of CsN is dynamically stable.

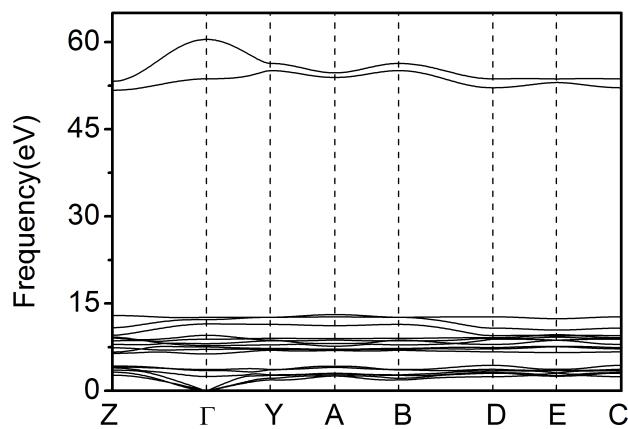


Fig. S5. Phonon dispersion curves of CsN₂ in the C2/m phase at 20 GPa. The absence of any imaginary frequency in the whole Brillouin zone demonstrated that C2/m structure of CsN₂ is dynamically stable.

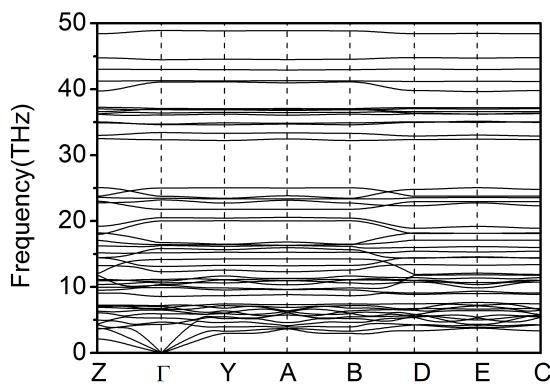


Fig. S6. Phonon dispersion curves of CsN₃ in the C2/m phase at 100 GPa. The absence of any imaginary frequency in the whole Brillouin zone demonstrated that C2/m structure of CsN₃ is dynamically stable.

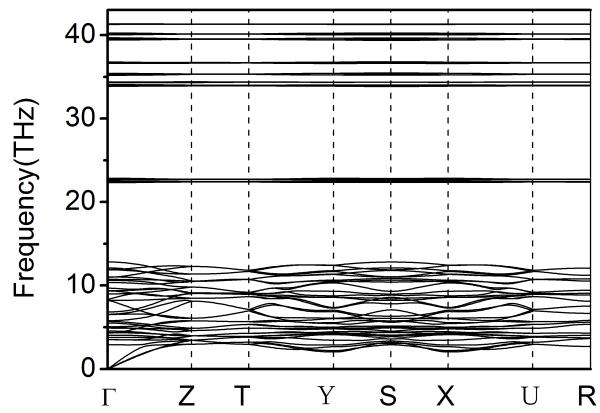


Fig. S7. Phonon dispersion curves of CsN_5 in the $Cmc2_1$ phase at 50 GPa. The absence of any imaginary frequency in the whole Brillouin zone demonstrated that $Cmc2_1$ structure of CsN_5 is dynamically stable.

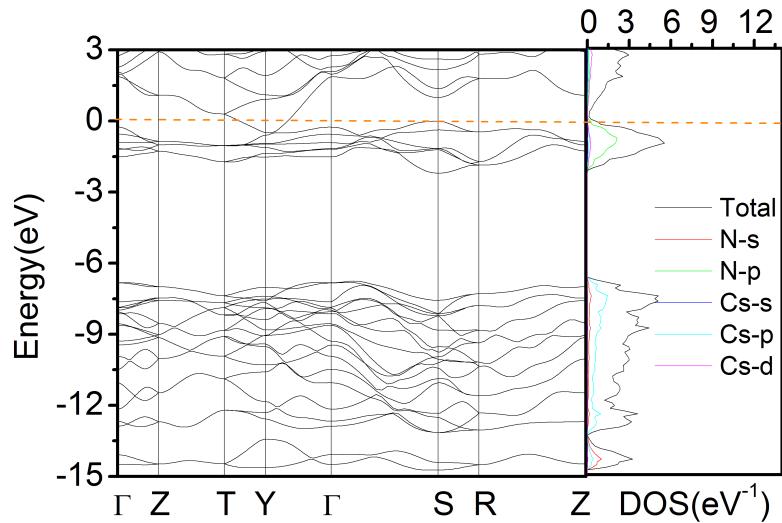


Fig. S8. Electronic band structure (left panel) and projected density of states (PDOS, right panel) of Cs_3N with $Cmcm$ symmetry at 50 GPa. The dashed line indicates the Fermi energy.

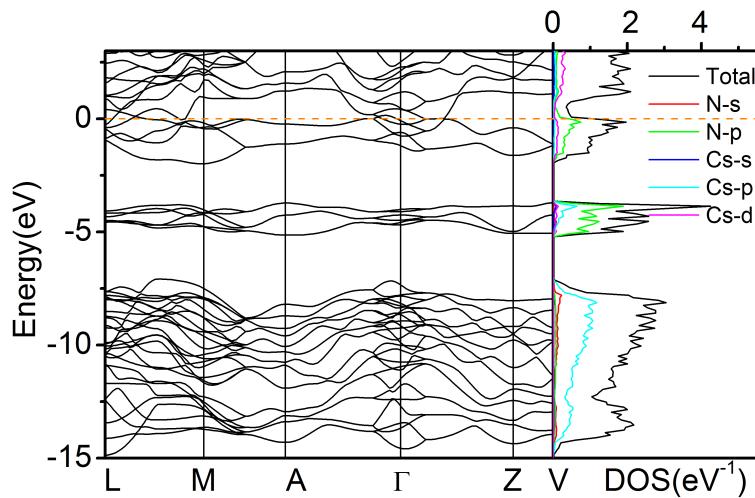


Fig. S9. Electronic band structure (left panel) and projected density of states (PDOS, right panel) of Cs_2N with $C2/m$ symmetry at 50 GPa. The dashed line indicates the Fermi energy.

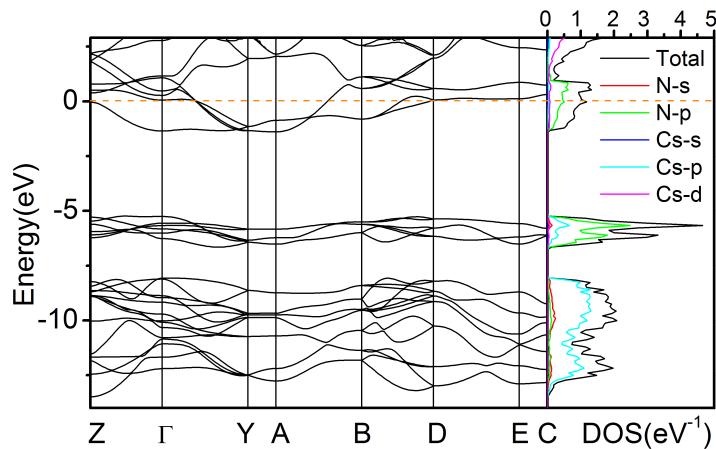


Fig. S10. Electronic band structure (left panel) and projected density of states (PDOS, right panel) of CsN with $C2/m$ symmetry at 20 GPa. The dashed line indicates the Fermi energy.

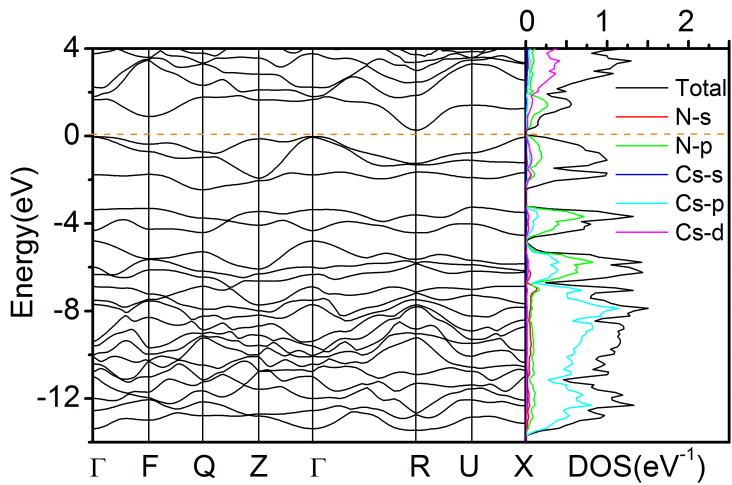


Fig. S11. Electronic band structure (left panel) and projected density of states (PDOS, right panel) of CsN with $P-1$ symmetry at 50 GPa. The dashed line indicates the Fermi energy.

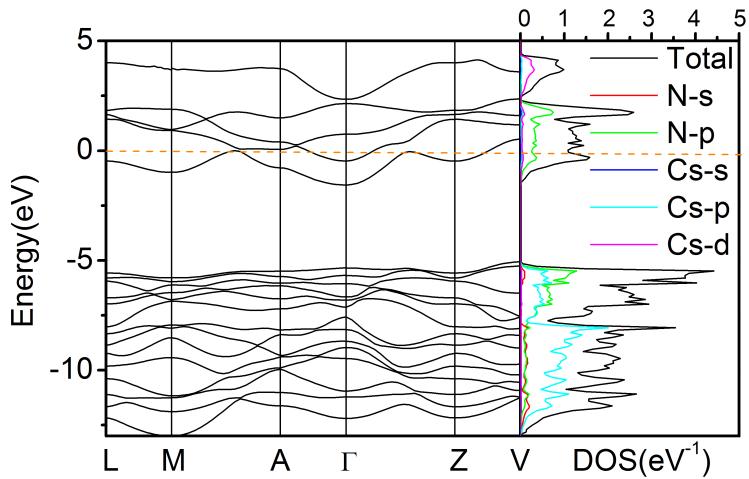


Fig. S12. Electronic band structure (left panel) and projected density of states (PDOS, right panel) of CsN_2 with $C2/m$ symmetry at 20 GPa. The dashed line indicates the Fermi energy.

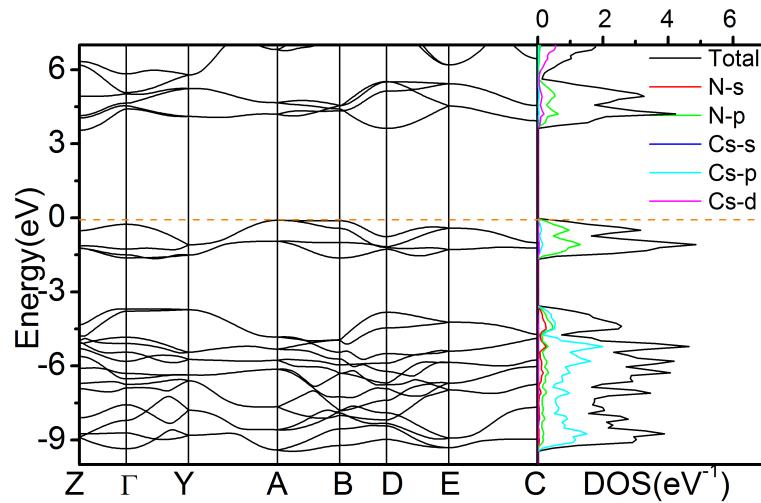


Fig. S13. Electronic band structure (left panel) and projected density of states (PDOS, right panel) of CsN_3 with $P2_1/m$ symmetry at 20 GPa. The dashed line indicates the Fermi energy.

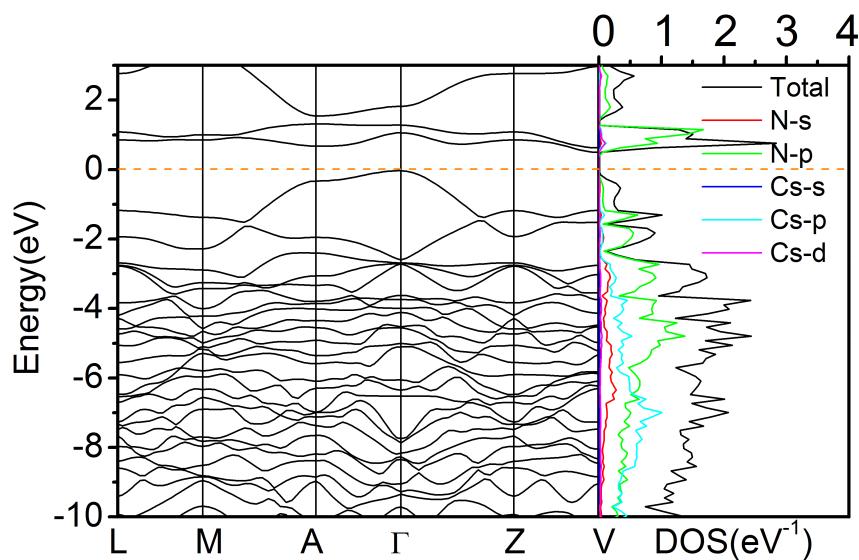


Fig. S14. Electronic band structure (left panel) and projected density of states (PDOS, right panel) of CsN_3 with $C2/m$ symmetry at 100 GPa. The dashed line indicates the Fermi energy.

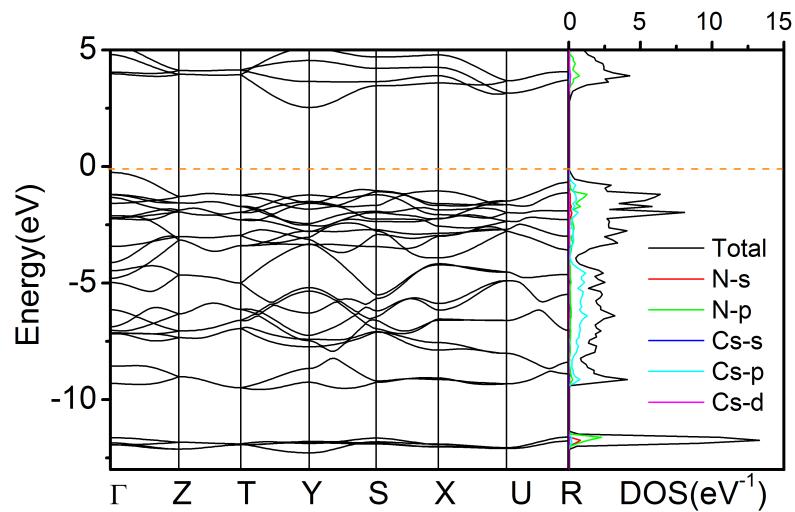


Fig. S15. Electronic band structure (left panel) and projected density of states (PDOS, right panel) of CsN_5 with $Cmc2_1$ symmetry at 50 GPa. The dashed line indicates the Fermi energy.

Supplementary Table

Table S1. Calculated structural parameters of various Cs-N compounds.

		Space group	Lattice Parameters (Å, °)	Atoms	Atomic coordinates (fractional)		
					X	Y	Z
Cs₃N (50 GPa)	<i>Cmcm</i>	<i>a</i> = 3.3911 <i>b</i> = 10.4641 <i>c</i> = 8.4242	Cs(8f)	0.00000	-0.13871	1.43349	
			Cs(4c)	0.00000	-0.57608	0.75000	
			N(4c)	0.00000	-0.26047	0.75000	
		$\alpha=\beta=\gamma=90.0000^\circ$					
Cs₂N (50 GPa)	<i>C2/m</i>	<i>a</i> = 10.8502 <i>b</i> = 3.3807 <i>c</i> = 8.2598	Cs(4i)	0.26018	0.50000	0.34453	
			Cs(4i)	0.91680	0.00000	0.10727	
			N(4i)	0.02903	0.50000	0.60525	
		$\alpha=\beta=90.0000^\circ$ $\gamma = 136.9505^\circ$					
CsN (20 GPa)	<i>C2/m</i>	<i>a</i> = 10.6125 <i>b</i> = 3.3835 <i>c</i> = 4.1495	Cs(4i)	0.35173	0.50000	0.80928	
			N(4i)	0.04403	0.50000	0.62581	
		$\alpha=\beta=90.0000^\circ$ $\gamma = 102.9287^\circ$					
CsN (50 GPa)	<i>P-1</i>	<i>a</i> = 4.9212 <i>b</i> = 4.9386 <i>c</i> = 5.3148	Cs(2i)	0.97935	0.76213	0.28208	
			Cs(2i)	0.38474	0.30542	0.30212	
			N(2i)	0.21542	0.75305	0.87954	
		$\alpha=74.9090^\circ$ $\beta=109.3728^\circ$ $\gamma=101.0377^\circ$	N(2i)	0.42382	0.88039	0.05554	
CsN₂ (20 GPa)	<i>C2/m</i>	<i>a</i> = 7.9105 <i>b</i> = 6.7235 <i>c</i> = 3.5422	Cs(4i)	0.71239	0.00000	0.96850	
			N(8g)	0.44999	-0.30627	0.60216	
		$\alpha=\gamma=90.0000^\circ$ $\beta=101.5493^\circ$					
CsN₂ (0 GPa)	<i>C2/c</i>	<i>a</i> = 11.07710 <i>b</i> = 6.7982 <i>c</i> = 5.9044	Cs(8f)	0.34184	-0.33396	0.21260	
			N(8f)	0.45355	0.06237	0.02036	
			N(8f)	0.45185	-0.20859	0.68566	
		$\alpha=\gamma=90.0000^\circ$ $\beta=77.8797^\circ$					
CsN₃ (0 GPa)	<i>I4/mcm</i>	<i>a</i> = <i>b</i> = 6.6930 <i>c</i> = 8.2040	Cs(4a)	0.50000	0.50000	0.25000	
			N(8h)	0.87427	0.37427	0.50000	
		$\alpha=\beta=\gamma=90.0000^\circ$	N(4d)	0.00000	0.50000	0.50000	
CsN₃	<i>C2/m</i>	<i>a</i> = 11.3067	Cs(4i)	0.38277	0.00000	0.73364	

(10 GPa)		$b = 5.4036$	Cs(4i)	0.77724	0.00000	0.65536
		$c = 4.9467$	N(8j)	0.14666	0.87834	0.90961
		$\alpha=\gamma=90.0000^\circ$	N(8j)	0.49380	0.61702	0.71962
		$\beta=73.2020^\circ$	N(8j)	0.42705	0.25219	0.20005
CsN₃	<i>P2₁/m</i>	$a = 3.5020$	Cs(2e)	0.05071	0.25000	0.19007
(20 GPa)		$b = 4.9299$	N(2e)	0.54949	0.25000	0.67681
		$c = 6.6482$	N(2e)	0.58104	0.75000	0.17041
		$\alpha=\gamma=90.0000^\circ$	N(2e)	0.29788	0.75000	0.46610
		$\beta=100.2791^\circ$				
CsN₃	<i>C2/m</i>	$a = 11.30670$	Cs(4i)	0.38277	0.00000	0.73364
(100 GPa)		$b = 5.4036$	Cs(4i)	0.77724	0.00000	0.65536
		$c = 4.9467$	N(8j)	0.14666	0.87834	0.90961
		$\alpha=\gamma=90.0000^\circ$	N(8j)	0.49380	0.61702	0.71962
		$\beta=73.202^\circ$	N(8j)	0.42705	0.25219	0.20005
CsN₅	<i>Cmc2₁</i>	$a = 10.457099$	Cs(4a)	0.00000	-0.87531	0.80441
(50 GPa)		$b = 9.506692$	Cs(4a)	0.00000	-0.37929	0.86663
		$c = 4.77148$	N(8b)	0.13918	-0.85348	0.29583
		$\alpha=\beta=\gamma=90.0000^\circ$	N(8b)	0.29969	-0.55046	0.65793
			N(8b)	-0.28006	-0.71207	0.95633
			N(8b)	0.16852	-0.34499	0.41872
			N(8b)	-0.18207	-0.55538	0.73533